



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 02:35 PM EDT

PDB ID : 1XRS / pdb_00001xrs
Title : Crystal structure of Lysine 5,6-Aminomutase in complex with PLP, cobalamin, and 5'-deoxyadenosine
Authors : Berkovitch, F.; Behshad, E.; Tang, K.H.; Enns, E.A.; Frey, P.A.; Drennan, C.L.
Deposited on : 2004-10-15
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

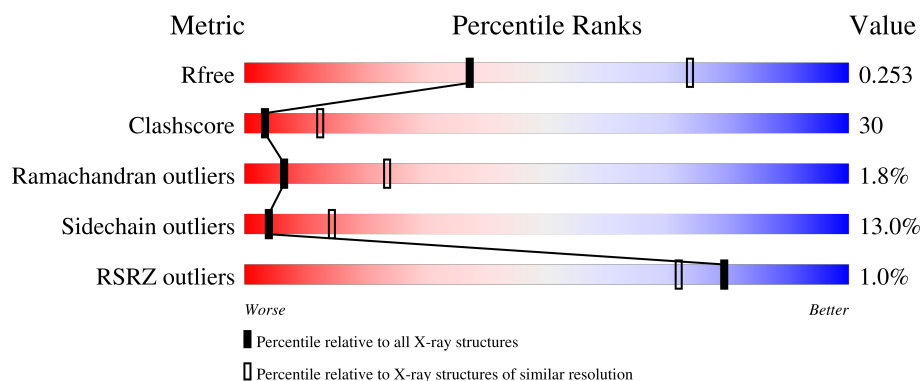
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

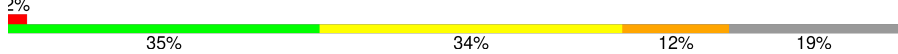
The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	516	 2% 50% 39% 10%
2	B	262	 2% 35% 34% 12% 19%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5797 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

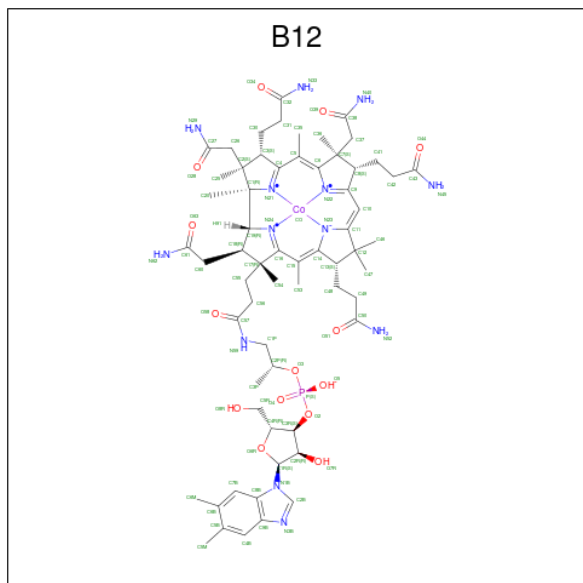
- Molecule 1 is a protein called D-lysine 5,6-aminomutase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4022	2551	671	775	25			

- Molecule 2 is a protein called D-lysine 5,6-aminomutase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1651	1040	277	325	9			

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



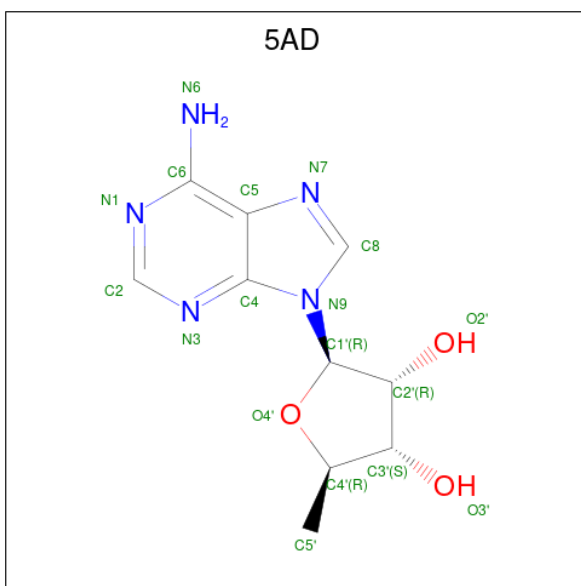
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

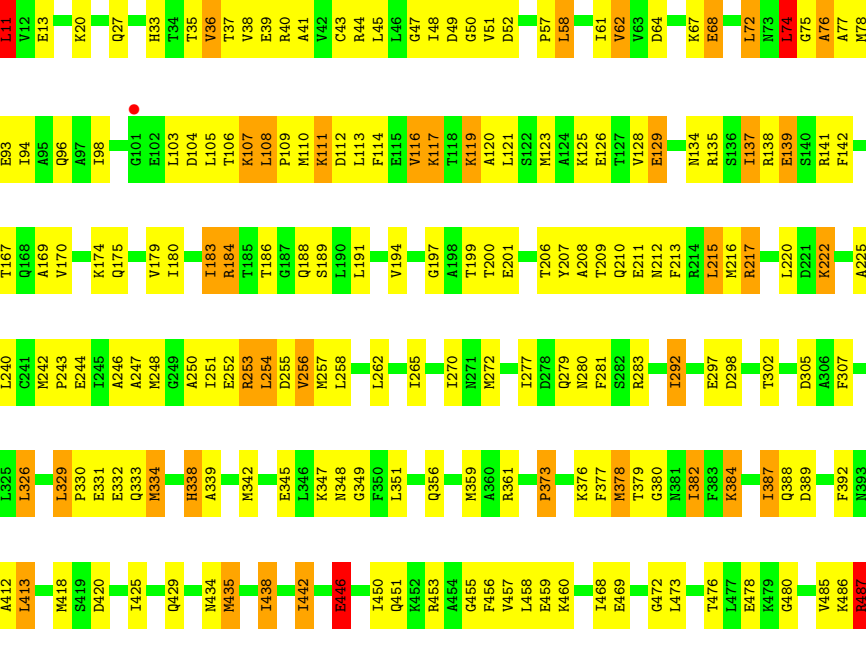
- Molecule 5 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			18	10	5	3		

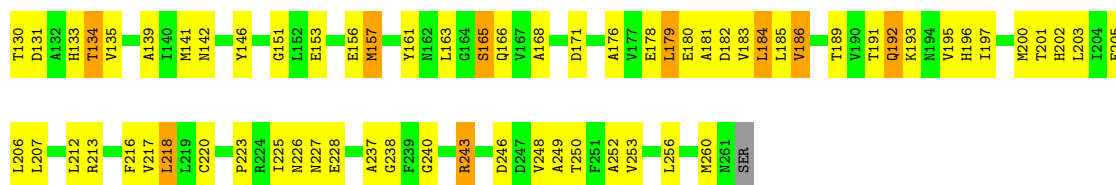
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain A: 



G497	L405	F318	C234	T159	H86	M1
V498	L406	I319	M236	G160	H87	E2
V499	L407	F322	M237	M161	G88	S3
S500	L409	G323	C238	I162	K89	K4
K501	T410	F324	G239	T166	E93	N10
D502	E411	A324	G240	G167	I94	L11
E503	A412	L325	L240	T168	A95	E13
H504	L413	G326	C241	A169	G96	E13
Y505	M418	L329	P242	V170	A97	K20
Y506	S419	P330	M243	K174	I98	
N507	D420	E331	E244	Q175	G101	Q27
P508	I425	M334	K248	V179	E102	H33
F509	Q429	H338	G249	I180	L103	T34
L512	M434	A339	T251	T183	D104	T35
H513	M435	E252	E252	I184	L105	V36
L514	I438	M342	K253	T185	T106	T37
M515	I442	E345	L254	G187	K107	V38
K516	E446	L346	D255	Q188	P109	E39
	I450	K347	V256	Q189	M110	R40
	Q451	N348	W257	S189	K111	A41
	K452	G349	L258	I190	D112	Y42
	R453	L351	L262	L191	F114	C43
	A454	Q356	L265	V194	E115	L46
	G455	M359	T270	G197	V116	G47
	F456	W271	K272	A198	K117	I48
	V457	R361	W272	T199	K119	D49
	L458	P373	L277	T209	A120	G50
	E459	K376	D278	Q210	T127	V62
	K460	F377	M280	E282	V128	V63
	I468	T378	F281	E283	E129	D64
	E469	M378	S282	E283	K67	
	Q472	G380	L292	T213	E68	
	L473	N381	L292	F214	L72	
	T476	L382	E297	L215	W73	
	E478	K384	D298	W216	L74	
	K479	I387	T302	R217	G75	
	G480	Q388	D305	L220	A76	
	V485	D389	A306	K221	M77	
	K486	F392	F307	K222	Y79	
	P488	N393	H311	A225	L80	
	G491	M394	T312	E226	A81	
	Q494	Q401	V313	G228	M82	
	L495	S316	L314	L231	A83	
	N496	W404	Q217	R232	V84	

- Chain B:
-
- 35% 34% 12% 19%
- MET SER SER GLY LEU TYR SER MET GLU LYS LYS PHE ASP LYS VAL LEU ASP LEU GLU ARG VAL GLN VAL SER LYS PRO TYR GLY ASP THR MET ASN ASP GLY K33 L36 S37 F38 T39 L40 P41 L42 F43 N44 M45 E46 Y49 E50 A51 A52 K53 Q54 L55 A56 L57 K58 M59 G60 L61 F62



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.70Å 99.70Å 168.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 2.80 49.85 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.85-2.80) 98.6 (49.85-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.49 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.199 , 0.262 0.191 , 0.253	Depositor DCC
R_{free} test set	2403 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5797	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, B12, 5AD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	2/4085 (0.0%)	1.25	38/5510 (0.7%)
2	B	0.81	1/1673 (0.1%)	1.26	18/2255 (0.8%)
All	All	0.82	3/5758 (0.1%)	1.25	56/7765 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	MET	SD-CE	-6.91	1.62	1.79
2	B	157	MET	SD-CE	-5.55	1.65	1.79
1	A	292	ILE	CA-CB	-5.42	1.47	1.54

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	62	GLU	N-CA-C	14.98	123.14	108.75
1	A	254	LEU	N-CA-C	-9.05	99.28	110.41
2	B	182	ASP	N-CA-C	-8.72	103.15	113.88
1	A	253	ARG	N-CA-C	8.46	120.80	110.91
1	A	175	GLN	N-CA-C	-8.11	103.36	113.18

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	TYR	Sidechain
1	A	505	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4022	0	4034	237	0
2	B	1651	0	1631	112	0
3	B	91	0	82	10	0
4	B	15	0	6	0	0
5	B	18	0	13	0	0
All	All	5797	0	5766	349	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

The worst 5 of 349 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:800:B12:C3R	3:B:800:B12:O2	1.64	1.44
2:B:192:GLN:HG3	2:B:193:LYS:H	1.03	1.10
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.18	1.08
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.23	1.03
2:B:189:THR:HG23	2:B:223:PRO:HG3	1.46	0.95

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/516 (100%)	471 (92%)	36 (7%)	7 (1%)	9	30
2	B	208/262 (79%)	184 (88%)	18 (9%)	6 (3%)	3	13
All	All	722/778 (93%)	655 (91%)	54 (8%)	13 (2%)	6	23

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	THR
1	A	111	LYS
1	A	446	GLU
2	B	192	GLN
2	B	44	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/429 (100%)	377 (88%)	52 (12%)	5	16
2	B	177/223 (79%)	150 (85%)	27 (15%)	3	10
All	All	606/652 (93%)	527 (87%)	79 (13%)	4	14

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	GLN
2	B	163	LEU
2	B	61	LEU
2	B	84	ASN
2	B	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	188	GLN
2	B	192	GLN
2	B	202	HIS
1	A	356	GLN
1	A	311	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PLP	B	801	2	15,15,16	5.52	8 (53%)	21,22,23	2.37	7 (33%)
5	5AD	B	500	-	20,20,20	1.11	1 (5%)	28,30,30	1.30	3 (10%)
3	B12	B	800	2	94,101,101	2.91	44 (46%)	149,166,166	2.50	44 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLP	B	801	2	-	1/6/6/8	0/1/1/1
5	5AD	B	500	-	-	0/4/20/20	0/3/3/3
3	B12	B	800	2	-	9/56/223/223	0/3/11/11

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	PLP	C5-C4	15.45	1.58	1.40
3	B	800	B12	O6R-C1R	9.17	1.63	1.42
4	B	801	PLP	C6-C5	7.54	1.52	1.37
3	B	800	B12	C4B-C5B	7.53	1.49	1.39
3	B	800	B12	C4B-C9B	7.50	1.51	1.40

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	800	B12	C19-N24-C16	14.65	123.31	107.29
3	B	800	B12	C9-N22-C6	10.28	117.65	105.28
3	B	800	B12	C1-C19-N24	7.60	114.70	106.25
4	B	801	PLP	O4P-P-O1P	-6.64	88.49	106.44
3	B	800	B12	O58-C57-C56	-5.92	111.29	122.02

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	800	B12	C14-C13-C48-C49
3	B	800	B12	C12-C13-C48-C49
3	B	800	B12	C2R-C1R-N1B-C8B
3	B	800	B12	O6R-C1R-N1B-C8B
3	B	800	B12	C42-C41-C8-C9

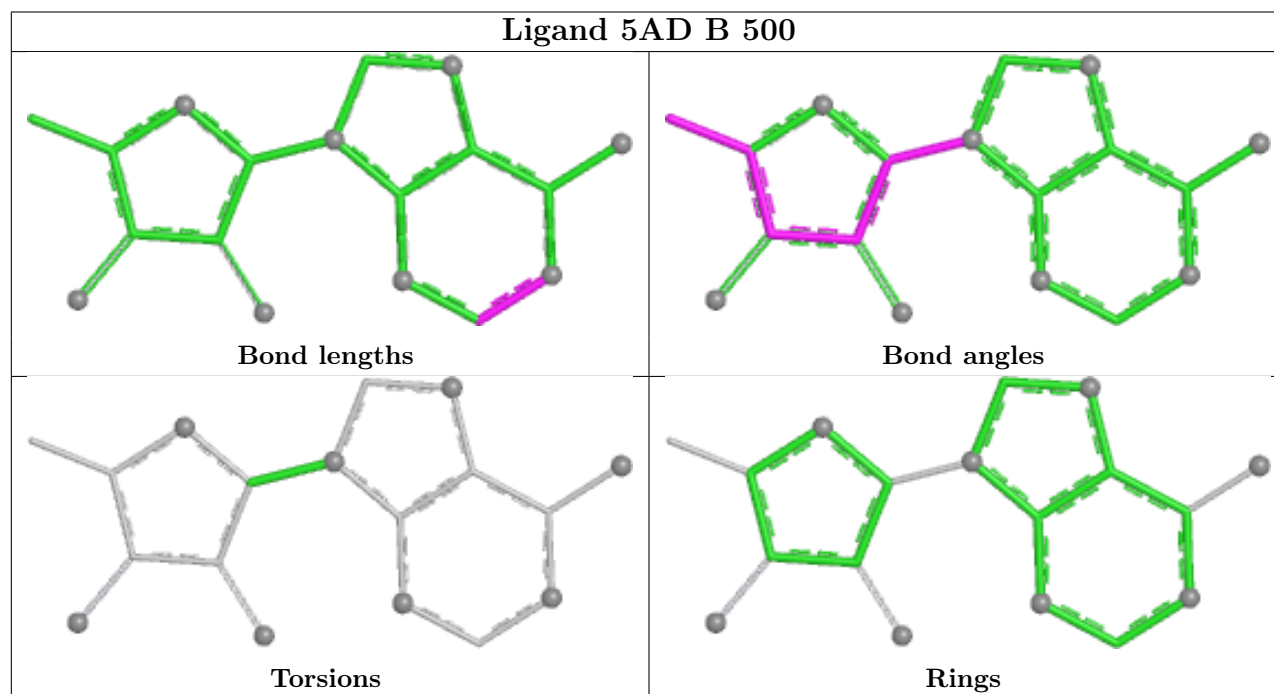
There are no ring outliers.

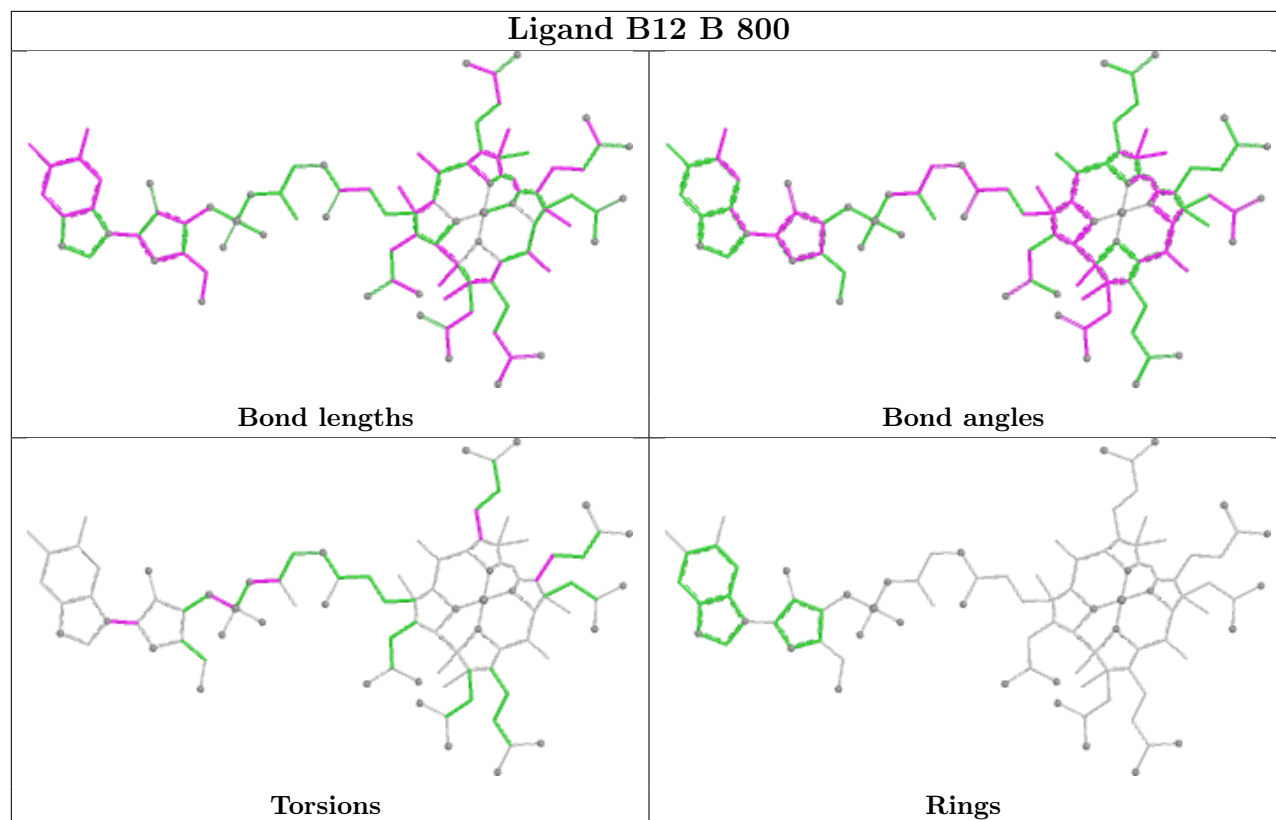
1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	800	B12	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	516/516 (100%)	-0.39	3 (0%) 85 80	9, 28, 54, 86	0
2	B	212/262 (80%)	-0.10	4 (1%) 66 57	12, 32, 74, 102	0
All	All	728/778 (93%)	-0.31	7 (0%) 79 72	9, 29, 61, 102	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	LEU	5.8
1	A	516	LYS	3.2
2	B	62	GLU	2.6
2	B	107	GLU	2.6
1	A	101	GLY	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

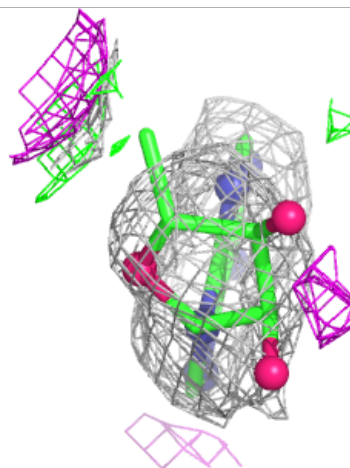
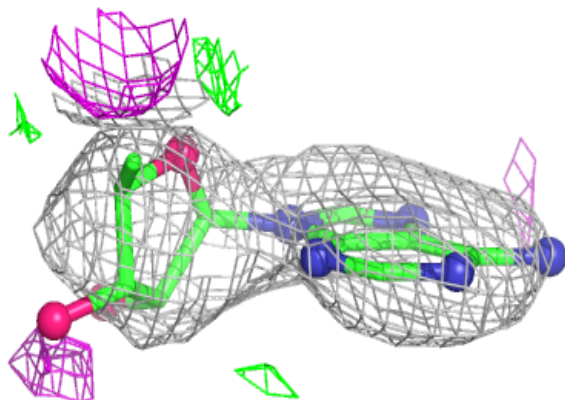
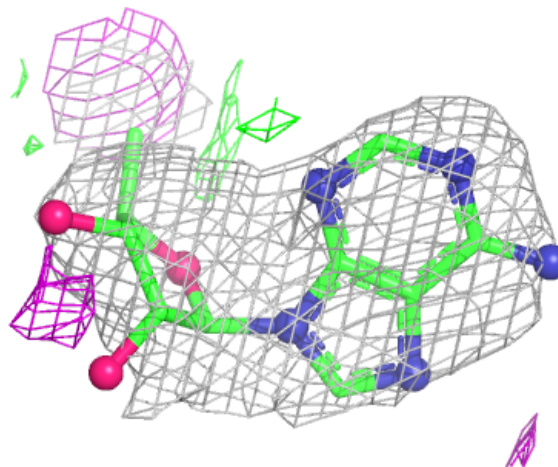
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	5AD	B	500	18/18	0.84	0.19	72,79,83,85	0
3	B12	B	800	91/91	0.92	0.11	0,30,48,55	0
4	PLP	B	801	15/16	0.97	0.07	22,25,30,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

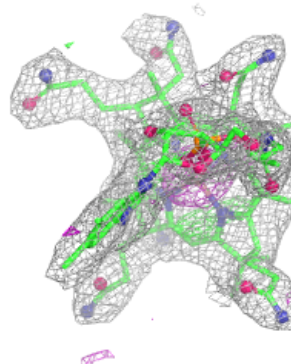
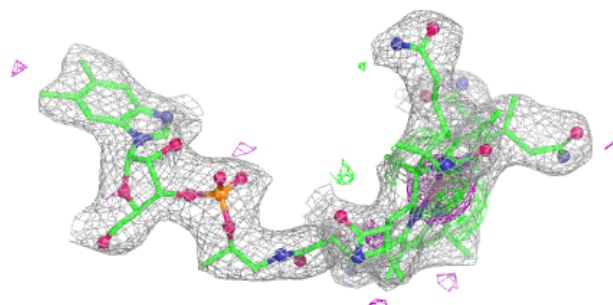
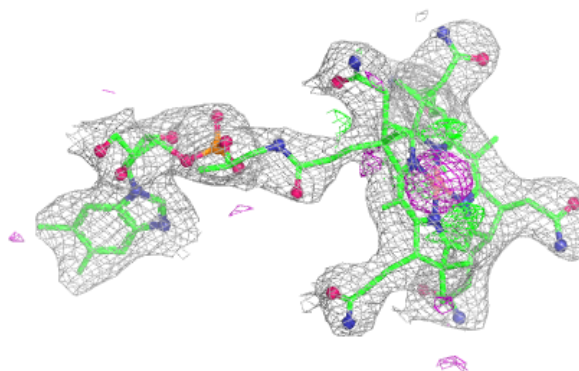
Electron density around 5AD B 500:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B12 B 800:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.